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Data-driven stochastic modeling of reaction initiation in granular energetic materials

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Modeling and simulation of thermal localization and reaction initiation in granular energetic materials under dynamic compaction is a formidable task. The main challenge lies in considering a wide range of multiphysics and multiscale phenomena while accounting for inevitable uncertainties in relevant quantities of interest. To quantify the probability of reaction initiation, we consider a random initial microstructure and study its effect on the probability distribution of the temperature using a multiscale two-phase granular compaction model. Finally, after deriving an unclosed equation for the joint PDF, we use a data-driven sparse identification method to learn an analytical form of the closure terms from Monte Carlo simulations. The results reveal a promising direction for data-driven coarse-graining in general.